

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: L. GGLWIM Examiner #: 77000 Date: 8/28/00
 Art Unit: 1713 Phone Number 306-5701 Serial Number: 09/761625
 Mail Box and Bldg/Room Location: CP3-9A11 Results Format Preferred (circle): PAPER DISK E-MAIL
CP3-9A11

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover-sheet, pertinent claims, and abstract.

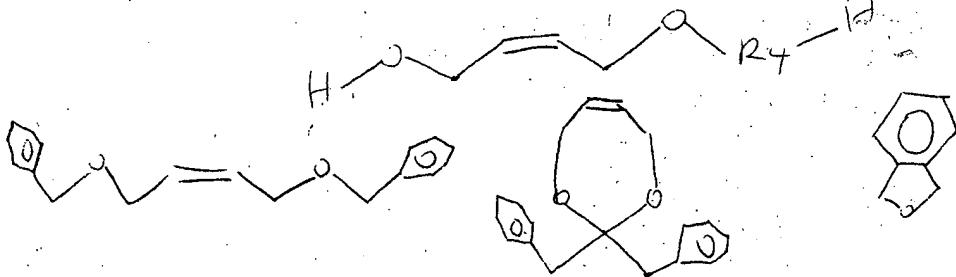
Title of Invention: Stabilization of Polymers after Synthesis
 Inventors (please provide full names): Qi Wang

Earliest Priority Filing Date: 3/99

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please Search for the compound S-01:
Claim 2 in any type of polymeric composition. Do Not limit the search to stabilizers

Focus on the following:



The end

STAFF USE ONLY

 Searcher: ED

Type of Search

Vendors and cost where applicable

NA Sequence (#)

STN

\$265.59

Searcher Phone #:

AA Sequence (#)

Dialog

Searcher Location:

Structure (#)

Questel/OFFP

Date Searcher Picked Up:

Bibliographic

DRI Link

Date Completed: 8-28-02

Litigation

Lexis/Nexis

Searcher Prep & Review Time: 5

Fulltext

Sequence Systems

Clerical Prep Time:

Patent Family

WWW/Internet

Online Time: 70

Other

Other (specify)

=> file reg
FILE 'REGISTRY' ENTERED AT 17:36:24 ON 28 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

=> d his

FILE 'LREGISTRY' ENTERED AT 16:31:23 ON 28 AUG 2002
L1 STR

FILE 'REGISTRY' ENTERED AT 16:33:26 ON 28 AUG 2002
L2 1 S L1

FILE 'LREGISTRY' ENTERED AT 16:33:43 ON 28 AUG 2002

FILE 'REGISTRY' ENTERED AT 16:48:16 ON 28 AUG 2002
L3 SCR 1016 OR 997
L4 SCR 1339 OR 1298
L5 SCR 1706 OR 1707
L6 SCR 1992 OR 2016 OR 2021 OR 2026 OR 1929 OR 1918
L7 13 S L1 AND L3 AND L4 AND L5 NOT L6
L8 1107 S L1 AND L3 AND L4 AND L5 NOT L6 FUL
SAV L8 EGW625C/A
E C18H20O2/MF
L9 2162 S E3
L10 11 S L9 AND L8
L11 232587 S ?BENZYL?/CNS
L12 3 S L10 AND L11
E C19H20O2/MF
L13 1526 S E3
L14 0 S L13 AND L8
L15 5149 S OCOC4/ESS
L16 1674 S OCOC4/ES
L17 159 S L8 AND (L15 OR L16)
L18 0 S L17 AND L11
L19 13 S L17 AND 3/NRS
E C8H8O/MF
L20 395 S E3

FILE 'LREGISTRY' ENTERED AT 17:02:15 ON 28 AUG 2002
L21 STR
L22 23 S L21

FILE 'REGISTRY' ENTERED AT 17:03:27 ON 28 AUG 2002
L23 57044 S 333.84.17/RID
L24 2 S L20 AND L23

FILE 'LREGISTRY' ENTERED AT 17:04:23 ON 28 AUG 2002
L25 STR

FILE 'REGISTRY' ENTERED AT 17:16:24 ON 28 AUG 2002
L26 0 S L25 SSS SAM SUB=L8
L27 27 S L25 SSS FUL SUB=L8
 SAV L27 EGW625D/A

FILE 'HCA' ENTERED AT 17:23:10 ON 28 AUG 2002
L28 1214958 S STABL? OR STABIL?
L29 593319 S POLYVINYL##(2A)CHLORIDE# OR POLY(2A)VINYL##(2A)CHLORIDE
L30 36 S L12
L31 146 S L24
L32 165 S L27
L33 3 S L30 AND L28
L34 2 S L30 AND L29
L35 3 S L33 OR L34
L36 12 S L31 AND L28
L37 4 S L31 AND L29
L38 13 S L36 OR L37
L39 7 S L32 AND L28
L40 2 S L32 AND L29
L41 7 S L39 OR L40

FILE 'REGISTRY' ENTERED AT 17:26:00 ON 28 AUG 2002
E POLYVINYL CHLORIDE/CN
L42 1 S E3
 E POLYETHYLENE/CN
L43 1 S E3
 E POLYPROPYLENE/CN
L44 1 S E3

FILE 'HCA' ENTERED AT 17:26:49 ON 28 AUG 2002
L45 251013 S L42 OR L43 OR L44
L46 2 S L30 AND L45
L47 3 S L31 AND L45
L48 2 S L32 AND L45
L49 3 S L35 OR L46
L50 13 S L38 OR L47
L51 7 S L41 OR L48

FILE 'REGISTRY' ENTERED AT 17:36:24 ON 28 AUG 2002
=> d l27 que stat
L1 STR
O×CH2×CH×CH×CH2×O
1 2 3 4 5 6

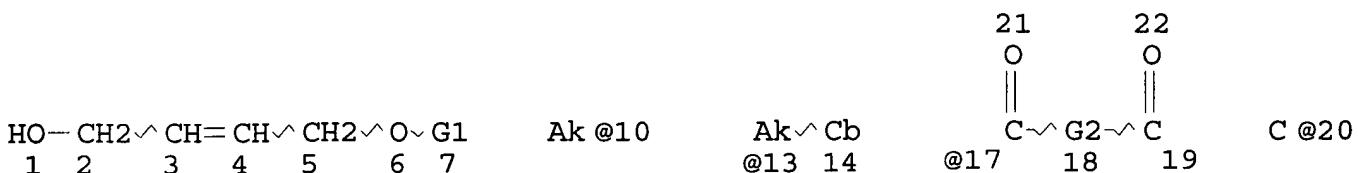
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE

L3 SCR 1016 OR 997
L4 SCR 1339 OR 1298
L5 SCR 1706 OR 1707
L6 SCR 1992 OR 2016 OR 2021 OR 2026 OR 1929 OR 1918
L8 1107 SEA FILE=REGISTRY SSS FUL L1 AND L3 AND L4 AND L5 NOT L6
L25 STR



VAR G1=10/13/17

REP G2=(1-8) 20

NODE ATTRIBUTES:

NSPEC IS RC AT 20
CONNECT IS E1 RC AT 10
CONNECT IS E2 RC AT 13
DEFAULT MLEVEL IS ATOM
GGCAT IS SAT AT 10
GGCAT IS SAT AT 13
GGCAT IS UNS AT 14
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X6 C AT 10

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L27 27 SEA FILE=REGISTRY SUB=L8 SSS FUL L25

100.0% PROCESSED 832 ITERATIONS
SEARCH TIME: 00.00.03

27 ANSWERS

```
=> file hca
FILE 'HCA' ENTERED AT 17:36:58 ON 28 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)
```

=> d 149 1-3 cbib abs hitstr hitind

L49 ANSWER 1 OF 3 HCA COPYRIGHT 2002 ACS

136:247398 Etherification method for producing benzyl ether derivatives of 2-butene-1,4-diols. Krishnamurti, Ramesh; Wang, Qi; Smolka, Thomas F. (Occidental Chemical Corporation, USA; Stephens, Dinah, H.). PCT Int. Appl. WO 2002022537 A2 20020321, 19 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-GB4036 20010910. PRIORITY: US 2000-PV231790 20000911.

AB A method for producing benzyl ethers of 2-butene-1,4-diols, useful as polymer **stabilizers** (no data), comprises reacting 2-butene-1,4-diols (e.g., 2-butene-1,4-diol) with benzyl chlorides (e.g., benzyl chloride) in the presence of an alkali (e.g., sodium hydroxide) or alk. earth metal hydroxide or carbonate, optionally in the presence of a phase-transfer catalyst (e.g., benzyltriethylammonium chloride) to produce mono- and/or di-benzyl ethers of 2-butene-1,4-diols [e.g., 1,4-bis(benzyloxy)-2-butene] and recovering at least a portion of at least one such benzene deriv.

IT 70677-94-0P, 1,4-Bis(benzyloxy)-2-butene
(etherification method for producing benzyl ether derivs. of 2-butene-1,4-diols)

RN 70677-94-0 HCA

CN Benzene, 1,1'-[2-butene-1,4-diylbis(oxymethylene)]bis- (9CI) (CA INDEX NAME)



IC ICM C07C041-00

CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 37, 45

IT 70677-94-0P, 1,4-Bis(benzyloxy)-2-butene 80885-30-9P
(etherification method for producing benzyl ether derivs. of 2-butene-1,4-diols)

L49 ANSWER 2 OF 3 HCA COPYRIGHT 2002 ACS

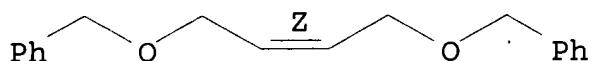
135:93426 **Stabilization** of polymers after exposure to oxidation and article manufacture. Wang, Qi (USA). U.S. Pat. Appl. Publ. US 20010007884 A1 20010712, 9 pp., Cont.-in-part of U. S. Ser. No. 272,843. (English). CODEN: USXXCO. APPLICATION: US 2001-761625 20010117. PRIORITY: US 1999-272843 19990319.

AB Polyvinyl chloride, polyvinylidene chloride, polycarbonate, polyethylene, polypropylene, polyamide, polyimide, polyether, polyester, or polyvinyl acetate contg. apprx.0.005-10 phr **stabilizer** are resistant to discoloring after exposure to oxidn. PVC contg. 1.34 g **stabilizer** phthalan had initial yellowness

value 17.5, after .gamma. radiation 31.9, and after aging 49.5, vs. 18.1, 50.2, and 75.5, resp., for a control without **stabilizer**.

IT 68972-96-3
 (stabilization of polymers after exposure to oxidn.)
 RN 68972-96-3 HCA
 CN Benzene, 1,1'-(2Z)-2-butene-1,4-diylbis(oxymethylene)bis- (9CI)
 (CA INDEX NAME)

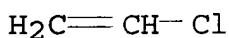
Double bond geometry as shown.



IT 9002-86-2, Poly(vinyl chloride)
) 9002-88-4, Polyethylene 9003-07-0,
 Polypropylene
 (stabilization of polymers after exposure to oxidn.)
 RN 9002-86-2 HCA
 CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4
 CMF C2 H3 Cl



RN 9002-88-4 HCA
 CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 74-85-1
 CMF C2 H4



RN 9003-07-0 HCA
 CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1
 CMF C3 H6

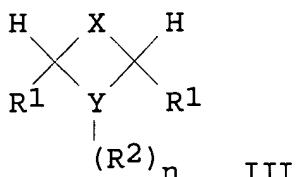
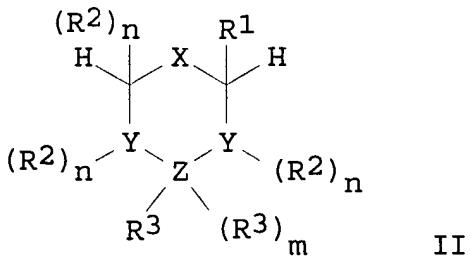
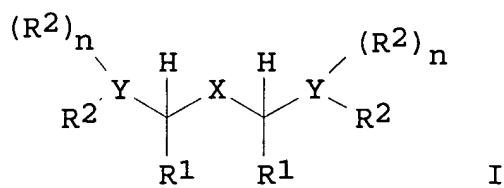


IC ICM C08K005-06
 ICS C08K005-46
 NCL 524083000
 CC 37-6 (Plastics Manufacture and Processing)
 ST discoloration prevention agents polymer; **PVC** phthalan
stabilizer; polyvinylidene chloride yellowing prevention;
polycarbonate yellowing prevention; **Polyethylene**
 yellowing prevention; **Polypropylene** yellowing prevention;
 polyamide yellowing prevention; polyimide yellowing prevention;
 polyether yellowing prevention; polyester yellowing prevention;
 polyvinyl acetate yellowing prevention
 IT Antioxidants
 Discoloration prevention agents
 Yellowing prevention
 (**stabilization** of polymers after exposure to oxidn.)
 IT Polyamides, uses
Polycarbonates, uses
 Polyesters, uses
 Polyethers, uses
 Polyimides, uses
Polyurethanes, uses
 (**stabilization** of polymers after exposure to oxidn.)
 IT 110-65-6, 2-Butyne-1,4-diol 332-77-4 496-14-0, Phthalan
 589-29-7, 1,4-Benzenedimethanol 1606-85-5, 1,4-Bis(2-hydroxy
 ethoxy)-2-butyne 2568-24-3 5417-32-3 10192-64-0 21285-46-1
 67461-24-9 **68972-96-3** 81028-03-7
 (**stabilization** of polymers after exposure to oxidn.)
 IT 9002-85-1, Poly(vinylidene chloride) **9002-86-2**,
Poly(vinyl chloride) **9002-88-4**
 , **Polyethylene** **9003-07-0**, **Polypropylene**
 9003-20-7, Poly(vinyl acetate)
 (**stabilization** of polymers after exposure to oxidn.)

L49 ANSWER 3 OF 3 HCA COPYRIGHT 2002 ACS

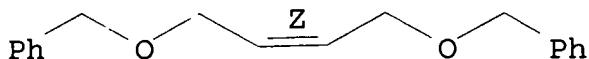
133:267624 **Stabilization** and discoloration prevention of
 polymers after exposure to oxidation and antioxidants therefor.
 Wang, Qi (Occidental Chemical Corporation, USA; Stephens, Dinah).
 PCT Int. Appl. WO 2000056812 A1 20000928, 37 pp. DESIGNATED STATES:
 W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
 CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN,
 IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,
 MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
 TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD,
 RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES,
 FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD,
 TG. (English). CODEN: PIIXD2. APPLICATION: WO 2000-GB247
 20000128. PRIORITY: US 1999-272843 19990319.

GI



- AB Poly(vinyl chloride), poly(vinylidene chloride), polycarbonates, polyethylene, polypropylene, polyamides, polyimides, polyethers, polyesters, or poly(vinyl acetate) contg. apprx. 0.005-10 phr of a **stabilizer** I, II, or III, where Z is C, P, Sn, Si, or B; X is -R1C:CR1-, ethynyl, (un)substituted benzene, pyridine, pyrimidine, triazine, furan, pyrrole, thiophene, or naphthalene ring; each Y is independently O, S, or N; each R is independently H, C1-24-alkyl, C6-24-aryl, C7-24-aralkyl; each R1 is independently R, OR, RCO, ROCO, ROCO2, PR2, P(OR)2, PR(OR), NR2, R2NCO, R2NCO2, SR, halogen, or two R1 groups can form a ring; each R2 is independently R, RCO, ROCO, P(OR)2, Sn(R)q(OR)3-q, SnRq(OCOR)3-q, Si(R)q(OR)3-q, BRq(OR)2-q, or two R2 groups can form a ring; each R3 is independently R, RCO, ROCO, ROCO2, OR, SR, NR2, OPR2, or OP(OR)2; m is 0 when Z is P or B and 1 when Z is Sn, Si, or C; n is 0 when Y is O or S and 1 when Y is N; p is 0-4; and q is 0-3 for the tin **stabilizers** and 0-2 for the boron **stabilizers**, with the proviso that in I, when X = -CH:CH-, Y = O and R2 = H, at least one of the R1 is not H; and in II, when X = -R1C:CR1-, Y = O and Z = C, then at least one of the R3 groups on Z is not H. Thus, a plaque from a compn. comprising PVC 150.00, stearic acid 0.30, Mark 152S 0.23, dioctyl phthalate 97.50, Drapex 6.8 15.00, and phthalan 1.34 g was irradiated with 50 kGy gamma-rays, and aged 48 h at 50.degree., giving yellowness 17.5 initially, 31.9 after radiation, and 49.5 after aging, compared with 18.1, 50.2, and 75.5, resp., without phthalan.
- IT 68972-96-3, cis-1,4-Bisbenzyloxy-2-butene 70677-94-0
 (stabilization and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)
- RN 68972-96-3 HCA
- CN Benzene, 1,1'-(2Z)-2-butene-1,4-diylbis(oxymethylene)]bis- (9CI)
 (CA INDEX NAME)

Double bond geometry as shown.



RN 70677-94-0 HCA
 CN Benzene, 1,1'-(2-butene-1,4-diylbis(oxymethylene)]bis- (9CI) (CA INDEX NAME)

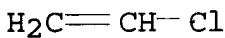


IT 9002-86-2, PVC 9002-88-4,
 Polyethylene 9003-07-0, Polypropylene
 (stabilization and discoloration prevention of polymers
 after exposure to oxidn. and antioxidants therefor)

RN 9002-86-2 HCA
 CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

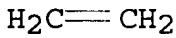
CRN 75-01-4
 CMF C2 H3 Cl



RN 9002-88-4 HCA
 CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

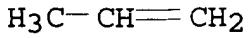
CRN 74-85-1
 CMF C2 H4



RN 9003-07-0 HCA
 CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1
 CMF C3 H6



IC ICM C08K005-00

=> d 150 1-13 cbib abs hitstr hitind

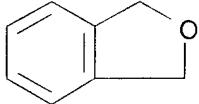
L50 ANSWER 1 OF 13 HCA COPYRIGHT 2002 ACS

137:78570 Conformational stabilization of phthalan: physical

origin of tiny ring-puckering barrier. Jeon, Sangmi; Choo, Jaebum; Kim, Sungwhan; Kwon, Younghui; Kim, Jin-Yeol; Lee, Young-Il; Chung,

Hoeil (Department of Chemistry, Hanyang University, Ansan, 425-791, S. Korea). Journal of Molecular Structure, 609(1-3), 159-167 (English) 2002. CODEN: JMSB4. ISSN: 0022-2860. Publisher: Elsevier Science B.V..

- AB The conformational property of phthalan has been investigated using ab initio calcn. and natural bond orbital (NBO) anal. methods. Geometry optimizations for the planar (C₂v) and puckered (Cs) conformers have been carried out using the HF, B3LYP, and MP methods, and the results indicate that this mol. has a tiny ring-puckering barrier. This barrier appears to be in good agreement with the previous exptl. result. NBO anal. shows that the tiny ring-puckering barrier is closely related to the MO interactions around the C-O bonds of the five-membered ring. The gas-phase IR and liq.-phase Raman spectra of phthalan and 1,3-benzodioxole have been recorded and analyzed in terms of C₂v symmetry. Vibrational frequency calcns. using the B3LYP method have also been performed to compare with the spectroscopic data. The B3LYP frequency calcns. do a reasonable job of estg. the frequencies.
- IT 496-14-0, Phthalan
(ab initio and NBO study on conformational **stabilization** of phthalan)
- RN 496-14-0 HCA
- CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



- CC 22-3 (Physical Organic Chemistry)
Section cross-reference(s): 73
- ST phthalan conformational **stabilization** ab initio NBO
- IT Density functional theory
(B3LYP; ab initio and NBO study on conformational **stabilization** of phthalan)
- IT Ab initio methods
Basis sets
Conformation
Conformational barrier
Conformational potential
Conformers
Electron correlation
Electron delocalization
HF MO (molecular orbital)
Hyperconjugation
MP2 (Moller-Plesset)
MP3 (Moller-Plesset)
MP4 (Moller-Plesset)
Molecular vibration
Natural bond orbital

Normal modes
QCISD(T) (molecular orbital)
Total energy
Vibrational frequency
(ab initio and NBO study on conformational **stabilization**
of phthalan)

IT IR spectra
Raman spectra
(exptl. and calcd.; ab initio and NBO study on conformational
stabilization of phthalan)

IT IR spectra
(far-IR; ab initio and NBO study on conformational
stabilization of phthalan)

IT IR spectra
(mid-IR; ab initio and NBO study on conformational
stabilization of phthalan)

IT Molecular structure
(optimized; ab initio and NBO study on conformational
stabilization of phthalan)

IT Molecular vibration
(puckering, ring puckering; ab initio and NBO study on
conformational **stabilization** of phthalan)

IT Potential barrier
(ring-puckering; ab initio and NBO study on conformational
stabilization of phthalan)

IT 496-11-7, Indan 496-14-0, Phthalan
(ab initio and NBO study on conformational **stabilization**
of phthalan)

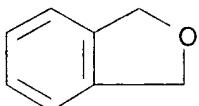
IT 274-09-9, 1,3-Benzodioxole
(ab initio and NBO study on conformational **stabilization**
of phthalan)

L50 ANSWER 2 OF 13 HCA COPYRIGHT 2002 ACS
135:332065 Thermoplastic resin composition. Kanayama, Satoshi;
Hatakeyama, Tatsuhiko; Miya, Shinya; Narita, Kenichi; Honma, Ken
(Japan). U.S. Pat. Appl. Publ. US 20010034419 A1 20011025, 20 pp.,
Cont.-in-part of WO1999JP 9904007. (English). CODEN: USXXCO.
APPLICATION: US 2001-768931 20010124. PRIORITY: JP 1998-212461
19980728; WO 1999-JP4007 19990727; JP 2000-15530 20000125; JP
2000-15531 20000125; JP 2000-15889 20000125; JP 2000-16033 20000125.

AB A thermoplastic resin compn. comprising: a transparent arom.
thermoplastic resin (a) and a copolyester resin (b) comprising at
least two kinds of dicarboxylic acid moieties and one kind of diol
moiety, 1 to 50 mol of the dicarboxylic acid moieties being a
naphthalenedicarboxylic acid moiety, the ratio of (a) to the
combined amt. of (a) and (b) being 55-99.99 by wt., and the ratio of
(b) being 0.01-45 by wt.

IT 496-14-0
(ionizing radiation **stabilizer**; thermoplastic resin
compn.)

RN 496-14-0 HCA
CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)

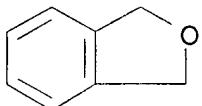


IC C08F020-00
 NCL 525439000
 CC 37-3 (Plastics Manufacture and Processing)
 Section cross-reference(s): 63
 IT Polyoxyalkylenes, uses
 /ionizing radiation **stabilizer**; thermoplastic resin
 compn.)
 IT Polycarbonates, uses
 Polyesters, uses
 (thermoplastic resin compn.)
 IT 80-48-8, Methyl p-toluene sulfonate 100-51-6, Benzyl alcohol, uses
 101-49-5, 2-Benzyl-1,3-dioxolane 102-04-5, Dibenzyl ketone
 103-41-3, Benzyl cinnamate 103-50-4, Dibenzyl ether 103-54-8,
 Cinnamyl acetate 104-54-1, Cinnamyl alcohol 110-88-3, Trioxane,
 uses 119-53-9, Benzoin 119-61-9, Benzophenone, uses 120-51-4,
 Benzyl benzoate 122-69-0, Cinnamyl cinnamate 123-63-7,
 Paraldehyde 300-57-2, Allylbenzene 462-95-3, Diethoxy methane
496-14-0 538-74-9, Dibenzylsulfide 574-09-4, Benzoin
 ethyl ether 620-32-6, Dibenzyl sulfone 621-08-9, Dibenzyl
 sulfoxide 622-22-0, 1,2-Dibenzylxyloxy ethane 640-60-8, Phenyl
 p-toluenesulfonate 649-15-0 696-59-3, 2,5-Dimethoxy
 tetrahydrofuran 772-00-9, 4-Phenyl-1,3-dioxane 945-51-7,
 Diphenyl sulfoxide 947-19-3, 1-Hydroxy cyclohexyl phenyl ketone
 1696-20-4 1746-13-0, Allyl phenyl ether 2550-40-5, Dicyclohexyl
 disulfide 2568-25-4, 4-Methyl-2-phenyl-1,3-dioxolane 6175-45-7,
 2,2-Diethoxy acetophenone 6543-04-0, 2,2'-Trimethylenebis[1,3-
 dioxolane 6770-38-3, 1,4-Bis-methoxymethyl benzene 9006-24-0,
 NIKANOL Y-50 17178-10-8 25322-69-4, Uniol D-2000 26403-62-3,
 Unisafe NKL-9520 56262-45-4, IUPILON FR-53 91528-47-1, Ethyl
 dimethyl aminobenzoate 151183-90-3, NIKANOL DS
 /ionizing radiation **stabilizer**; thermoplastic resin
 compn.)

L50 ANSWER 3 OF 13 HCA COPYRIGHT 2002 ACS
 135:93426 **Stabilization** of polymers after exposure to
 oxidation and article manufacture. Wang, Qi (USA). U.S. Pat. Appl.
 Publ. US 20010007884 A1 20010712, 9 pp., Cont.-in-part of U. S. Ser.
 No. 272,843. (English). CODEN: USXXCO. APPLICATION: US
 2001-761625 20010117. PRIORITY: US 1999-272843 19990319.
 AB **Polyvinyl chloride**, polyvinylidene
 chloride, **polycarbonate**, **polyethylene**,
 polypropylene, polyamide, polyimide, polyether, polyester,
 or polyvinyl acetate contg. .aprx.0.005-10 phr **stabilizer**
 are resistant to discoloring after exposure to oxidn. PVC
 contg. 1.34 g **stabilizer** phthalan had initial yellowness

value 17.5, after .gamma. radiation 31.9, and after aging 49.5, vs. 18.1, 50.2, and 75.5, resp., for a control without **stabilizer**.

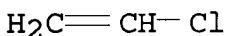
IT 496-14-0, Phthalan
 (stabilization of polymers after exposure to oxidn.)
 RN 496-14-0 HCA
 CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



IT 9002-86-2, Poly(vinyl chloride)
) 9002-88-4, Polyethylene 9003-07-0,
 Polypropylene
 (stabilization of polymers after exposure to oxidn.)
 RN 9002-86-2 HCA
 CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

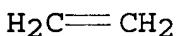
CRN 75-01-4
 CMF C2 H3 Cl



RN 9002-88-4 HCA
 CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

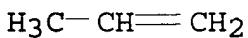
CRN 74-85-1
 CMF C2 H4



RN 9003-07-0 HCA
 CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1
 CMF C3 H6



IC ICM C08K005-06

NCL ICS C08K005-46
 524083000

CC 37-6 (Plastics Manufacture and Processing)

ST discoloration prevention agents polymer; PVC phthalan
stabilizer; polyvinylidene chloride yellowing prevention;
polycarbonate yellowing prevention; **Polyethylene**
 yellowing prevention; **Polypropylene** yellowing prevention;
 polyamide yellowing prevention; polyimide yellowing prevention;
 polyether yellowing prevention; polyester yellowing prevention;
 polyvinyl acetate yellowing prevention

IT Antioxidants
 Discoloration prevention agents
 Yellowing prevention
 (**stabilization** of polymers after exposure to oxidn.)

IT Polyamides, uses
Polycarbonates, uses
 Polyesters, uses
 Polyethers, uses
 Polyimides, uses
Polyurethanes, uses
 (**stabilization** of polymers after exposure to oxidn.)

IT 110-65-6, 2-Butyne-1,4-diol 332-77-4 **496-14-0**, Phthalan
 589-29-7, 1,4-Benzenedimethanol 1606-85-5, 1,4-Bis(2-hydroxy
 ethoxy)-2-butyne 2568-24-3 5417-32-3 10192-64-0 21285-46-1
 67461-24-9 68972-96-3 81028-03-7
 (**stabilization** of polymers after exposure to oxidn.)

IT 9002-85-1, Poly(vinylidene chloride) **9002-86-2**,
Poly(vinyl chloride) **9002-88-4**
Polyethylene **9003-07-0**, **Polypropylene**
 9003-20-7, Poly(vinyl acetate)
 (**stabilization** of polymers after exposure to oxidn.)

L50 ANSWER 4 OF 13 HCA COPYRIGHT 2002 ACS

134:326142 Thermal Reactions of Isodihydrobenzofuran: Experimental Results and Computer Modeling. Lifshitz, Assa; Suslensky, Aya; Tamburu, Carmen (Department of Physical Chemistry, The Hebrew University of Jerusalem, Jerusalem, 91904, Israel). Journal of Physical Chemistry A, 105(13), 3148-3157 (English) 2001. CODEN: JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.

AB The thermal reactions of isodihydrobenzofuran (phthalan) were studied behind reflected shock waves in a single pulse shock tube over the temp. range 1050-1300 K and overall densities of .aprx.3 .times. 10⁻⁵ mol/cm³. The total decompr. rate, expressed as a first-order rate const., is 1012.10 exp(-53.7 .times. 10³/RT) s⁻¹, where R is in given units of cal/(K mol). One isomerization product, o-tolualdehyde [kisomerization] = 1016.50 exp (-80.5 .times. 10³/RT) s⁻¹, and products resulting from unimol. cleavage of the furan ring were obtained under shock heating. Carbon monoxide and toluene are the products of the highest concn. Isobenzofuran is obtained by a 1,6-H₂ elimination from the furan ring with a rate const. k = 1013.78 exp(-70.0 .times. 10³/RT) s⁻¹. In addn., benzene, ethylbenzene, styrene, ethylene, methane, and

acetylene were found in the postshock mixts. Trace quantities of allene and propyne were also found. In addn. to H-atom ejection from the furan ring, it is believed that phthalan decompns. via two unimol. reactions that involve cleavage of the furan ring. One reaction yields **stable** products, phthalan .fwdarw.

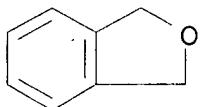
C₆H₅-CH₃ + CO [k = 1014.11 exp(-67.0 .times. 103/RT) s-1], and one decompn. yields unstable intermediates which are responsible for the propagation of free radical reactions in the system, phthalan .fwdarw. HCO.bul. + C₆H₅-CH₂.bul. (k = 1016.6 exp(-78.0 .times. 103/RT) s-1). A reaction scheme contg. 26 species and 49 elementary reactions was constructed, and computer modeling was performed in 25 K intervals over the range 1050-1300 K. The agreement between the exptl. and the calcd. yields is reasonable. Differences and similarities in the thermal behavior of isodihydrobenzofuran, dihydrobenzofuran, 2,3-dihydrofuran, and 2,5-dihydrofuran and the effect of fused benzene ring are discussed.

IT 496-14-0, Phthalan

(exptl. results and computer modeling of thermal reactions of isodihydrobenzofuran behind reflected shock waves)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 22-9 (Physical Organic Chemistry)

IT 496-14-0, Phthalan

(exptl. results and computer modeling of thermal reactions of isodihydrobenzofuran behind reflected shock waves)

L50 ANSWER 5 OF 13 HCA COPYRIGHT 2002 ACS

133:267624 **Stabilization** and discoloration prevention of

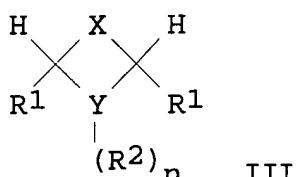
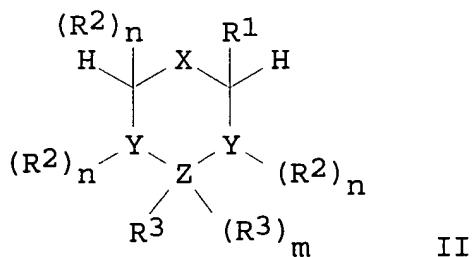
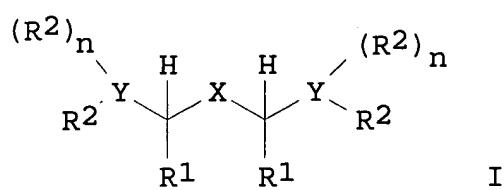
polymers after exposure to oxidation and antioxidants therefor.

Wang, Qi (Occidental Chemical Corporation, USA; Stephens, Dinah).

PCT Int. Appl. WO 2000056812 A1 20000928, 37 pp. DESIGNATED STATES:

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN,
IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,
MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD,
RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES,
FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD,
TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-GB247
20000128. PRIORITY: US 1999-272843 19990319.

GI



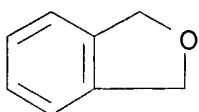
AB Poly(vinyl chloride), poly(vinylidene chloride), polycarbonates, polyethylene, polypropylene, polyamides, polyimides, polyethers, polyesters, or poly(vinyl acetate) contg. .apprx.0.005-10 phr of a **stabilizer** I, II, or III, where Z is C, P, Sn, Si, or B; X is -R1C:CR1-, ethynyl, (un)substituted benzene, pyridine, pyrimidine, triazine, furan, pyrrole, thiophene, or naphthalene ring; each Y is independently O, S, or N; each R is independently H, C1-24-alkyl, C6-24-aryl, C7-24-aralkyl; each R1 is independently R, OR, RCO, ROCO, ROCO₂, PR₂, P(OR)₂, PR(OR), NR₂, R₂NCO, R₂NCO₂, SR, halogen, or two R1 groups can form a ring; each R2 is independently R, RCO, ROCO, P(OR)₂, Sn(R)q(OR)_{3-q}, SnRq(OCOR)_{3-q}, Si(R)q(OR)_{3-q}, BRq(OR)_{2-q}, or two R2 groups can form a ring; each R3 is independently R, RCO, ROCO, ROCO₂, OR, SR, NR₂, OPR₂, or OP(OR)₂; m is 0 when Z is P or B and 1 when Z is Sn, Si, or C; n is 0 when Y is O or S and 1 when Y is N; p is 0-4; and q is 0-3 for the tin **stabilizers** and 0-2 for the boron **stabilizers**, with the proviso that in I, when X = -CH:CH-, Y = O and R2 = H, at least one of the R1 is not H; and in II, when X = -R1C:CR1-, Y = O and Z = C, then at least one of the R3 groups on Z is not H. Thus, a plaque from a compn. comprising PVC 150.00, stearic acid 0.30, Mark 152S 0.23, dioctyl phthalate 97.50, Drapex 6.8 15.00, and phthalan 1.34 g was irradiated with 50 kGy .gamma.-rays, and aged 48 h at 50.degree., giving yellowness 17.5 initially, 31.9 after radiation, and 49.5 after aging, compared with 18.1, 50.2, and 75.5, resp., without phthalan.

IT 496-14-0, Phthalan

(**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



IT 9002-86-2, PVC 9002-88-4,
Polyethylene 9003-07-0, Polypropylene
 (stabilization and discoloration prevention of polymers
 after exposure to oxidn. and antioxidants therefor)

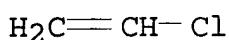
RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4

CMF C2 H3 Cl



RN 9002-88-4 HCA

CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 74-85-1

CMF C2 H4



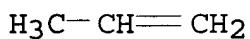
RN 9003-07-0 HCA

CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1

CMF C3 H6



IC ICM C08K005-00

ICS C08K005-053; C08K005-15; C08K005-06

CC 37-6 (Plastics Manufacture and Processing)

ST antioxidant yellowing prevention polymer; **PVC** phthalan
 antioxidant gamma radiation; polyolefin antioxidant yellowing
 prevention; vinyl compd polymer antioxidant yellowing prevention;
polycarbonate antioxidant yellowing prevention;
Polyurethane antioxidant yellowing prevention; polyamide
 antioxidant yellowing prevention; polyimide antioxidant yellowing

- IT prevention; polyether antioxidant yellowing prevention; polyester antioxidant yellowing prevention
- IT Yellowing prevention
- IT Yellowing prevention
(agents; **stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)
- IT Antioxidants
(**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)
- IT Polyamides, uses
- IT Polycarbonates, uses
- IT Polyesters, uses
- IT Polyethers, uses
- IT Polyimides, uses
- IT Polyurethanes, uses
(**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)
- IT Discoloration prevention agents
- IT Discoloration prevention agents
(yellowing; **stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)
- IT 110-64-5, 2-Butene-1,4-diol 110-65-6, 2-Butyne-1,4-diol
332-77-4, 2,5-Dimethoxy-2,5-dihydrofuran **496-14-0**,
Phthalan 589-29-7, 1,4-Benzenedimethanol 1606-85-5,
1,4-Bis(2-hydroxyethoxy)-2-butyne 2568-24-3, 4,7-Dihydro-2-phenyl-
1,3-dioxepin 10192-64-0 21285-46-1 67461-24-9 68972-96-3,
cis-1,4-Bisbenzyloxy-2-butene 70677-94-0 81028-03-7,
cis-4-Benzylbenzoate
(**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)
- IT 9002-85-1, Poly(vinylidene chloride) **9002-86-2**,
PVC **9002-88-4**, Polyethylene
9003-07-0, Polypropylene 9003-20-7, Poly(vinyl acetate)
(**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

L50 ANSWER 6 OF 13 HCA COPYRIGHT 2002 ACS

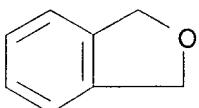
132:63957 Experimental determination of the antiaromaticity of cyclobutadiene. Deniz, Ashok A.; Peters, Kevin S.; Snyder, Gary J. (Dep. Chem., Univ. Chicago, Chicago, IL, 60637, USA). Science (Washington, D. C.), 286(5442), 1119-1122 (English) 1999. CODEN: SCIEAS. ISSN: 0036-8075. Publisher: American Association for the Advancement of Science.

AB Photoacoustic calorimetry was used to quantify the antiaromaticity of 1,3-cyclobutadiene (CBD) by measuring the heat release accompanying its formation via photofragmentation of a polycyclic precursor. In combination with quantum yield measurements and thermochem. calcns., this measurement provides an enthalpy of formation for CBD of 114 .+- . 11 (2.sigma.) kilocalories per mol (kcal/mol). The extraordinary reactivity of this prototypical antiarom. hydrocarbon had previously made its heat of formation

inaccessible except by theor. calcns. Relative to a hypothetical strainless, conjugated diene ref., CBD is destabilized by a total of 87 kcal/mol, 32 kcal/mol of which can be attributed to ring strain and 55 kcal/mol to antiaromaticity (compared with 21 kcal/mol for the arom. **stabilization** of benzene). Relative to a ref. with isolated double bonds, CBD's antiaromaticity is 48 kcal/mol (compared with 32 kcal/mol for the aromaticity of benzene).

IT 496-14-0, Phthalan
(formation heat; exptl. detn. of antiaromaticity of cyclobutadiene)

RN 496-14-0 HCA
CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 22-13 (Physical Organic Chemistry)
IT Stabilization energy

(isodesmic, homodesmic and; exptl. detn. of antiaromaticity of cyclobutadiene)

IT 496-14-0, Phthalan
(formation heat; exptl. detn. of antiaromaticity of cyclobutadiene)

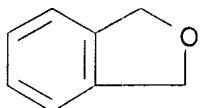
L50 ANSWER 7 OF 13 HCA COPYRIGHT 2002 ACS

125:142504 Electron-Transfer-Induced Reductive Cleavage of Phthalans: Reactivity and Synthetic Applications. Azzena, Ugo; Demartis, Salvatore; Melloni, Giovanni (Dipartimento di Chimica, Universita di Sassari, Sassari, I-07100, Italy). Journal of Organic Chemistry, 61(15), 4913-4919 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB The behavior of phthalan (1,3-dihydroisobenzofuran) was investigated under conditions of electron transfer from alkali metals in aprotic solvents. Reaction with lithium in the presence of a catalytic amt. of naphthalene in THF led to the reductive cleavage of an arylmethyl carbon-oxygen bond, with formation of a **stable** dilithium compd. Trapping of this intermediate with several electrophiles (alkyl halides, carbonyl derivs., CO₂) was successful. The extension of this procedure to several substituted phthalans was investigated, and the regiochem. as well as the synthetic usefulness of these reactions are discussed.

IT 496-14-0, Phthalan
(electron-transfer-induced reductive cleavage of phthalan derivs.)

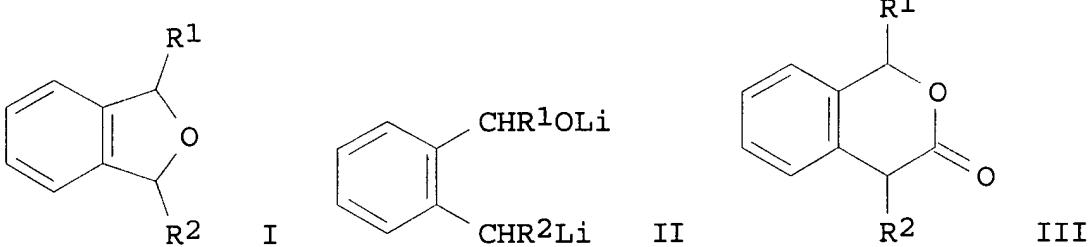
RN 496-14-0 HCA
CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



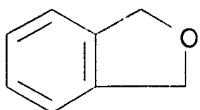
CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 22, 25
 IT 87-41-2, Phthalide 171-80-2, Spiro[cyclohexane-1,1'-phthalan]
496-14-0, Phthalan 7111-66-2 35185-96-7,
 1,4-Epoxy-1,2,3,4-tetrahydronaphthalene 42502-56-7, Isobenzofuran,
 1,3-dihydro-1,1-dimethyl
 (electron-transfer-induced reductive cleavage of phthalan
 derivs.)

L50 ANSWER 8 OF 13 HCA COPYRIGHT 2002 ACS
 124:55746 Reductive electrophilic substitution of phthalans and ring
 expansion to isochroman derivatives. Azzena, Ugo; Demartis,
 Salvatore; Fiori, Maria Giovanna; Melloni, Giovanni; Pisano, Luisa
 (Dip. Chim., Univ. di Sassari, Sassari, I-07100, Italy).
Tetrahedron Letters, 36(44), 8123-6 (English) 1995. CODEN: TELEAY.
 ISSN: 0040-4039. OTHER SOURCES: CASREACT 124:55746. Publisher:
 Elsevier.

GI

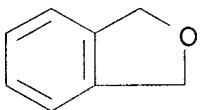


AB Reductive cleavage of phthalans I (R1 = H, R2 = H, Ph; R1R2 = CH2CH2) with Li and a catalytic amt. of naphthalene forms
 stable arom. dilithium compds. II, which undergo ring
 closure with CO2 to form isochromans III in yields >40%. II react
 with various alkyl halides, aldehydes and ketones to form
 o-substituted benzyl alcs. in yields > 60%.
 IT **496-14-0**, Phthalan
 (reductive electrophilic substitution of phthalans and ring
 expansion to isochromanone derivs.)
 RN 496-14-0 HCA
 CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
 IT 100-52-7, Benzaldehyde, reactions 119-61-9, Benzophenone,
 reactions 496-14-0, Phthalan 630-19-3,
 2,2-Dimethylpropionaldehyde 7111-66-2, Isobenzofuran,
 1,3-dihydro,1-phenyl- 35185-96-7
 (reductive electrophilic substitution of phthalans and ring
 expansion to isochromanone derivs.)

L50 ANSWER 9 OF 13 HCA COPYRIGHT 2002 ACS
 117:25733 Cobalt-catalyzed oxidation of ethers using oxygen. Li, Pei;
 Alper, Howard (Ottawa-Carleton Chem. Inst., Univ. Ottawa, Ottawa,
 ON, K1N 6N5, Can.). J. Mol. Catal., 72(2), 143-52 (English) 1992.
 CODEN: JMCADS. ISSN: 0304-5102. OTHER SOURCES: CASREACT 117:25733.
 AB Cobalt(II) chloride-catalyzed oxidn. of cyclic ethers with oxygen in
 1,2-dimethoxyethane gives the corresponding lactones in reasonable
 to excellent yields. Oxidn. of acyclic alkyl benzyl ethers affords
 the corresponding esters in yields which are dependent on the
 stability of alkyl radicals. The more stable the
 alkyl radical, the lower the yield of the formed ester. Oxidn. of
 acyclic alkyl and heterocyclic ethers is also described. A radical
 mechanism is proposed involving participation of superoxocobalt.
 IT 496-14-0
 (autoxidn. of, mechanism of catalytic)
 RN 496-14-0 HCA
 CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 22-7 (Physical Organic Chemistry)
 IT 103-50-4, Benzyl ether 109-99-9, reactions 142-96-1 493-05-0,
 Isochroman 496-14-0 538-86-3 539-30-0, Benzylethyl
 ether 946-80-5, Benzylphenyl ether 1612-65-3 1708-29-8,
 2,5-Dihydrofuran
 (autoxidn. of, mechanism of catalytic)

L50 ANSWER 10 OF 13 HCA COPYRIGHT 2002 ACS
 96:19300 Possible interactions of cyclobutadiene with by-products in
 inert matrix isolation studies. Fraga, Serafin (Dep. Chem., Univ.
 Alberta, Edmonton, AB, T6G 2G2, Can.). Tetrahedron Lett., 22(35),
 3343-6 (English) 1981. CODEN: TELEAY. ISSN: 0040-4039.
 AB A theor. study is reported of the complexes which may be formed by
 the in situ generation of cyclobutadiene with by-products in inert

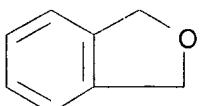
matrixes. Stable complexes are formed between cyclobutadiene and CO, HCN, phthalan, CO₂, C₆H₆, and cyclobutadiene, though the stabilization energies are small (-8.4 to -2.0 kJ).

IT 496-14-0

(interaction of, with cyclobutadiene in inert matrixes, theor. calcn. of)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 22-2 (Physical Organic Chemistry)

IT 71-43-2, reactions 74-90-8, properties 124-38-9, reactions

496-14-0 630-08-0, reactions

(interaction of, with cyclobutadiene in inert matrixes, theor. calcn. of)

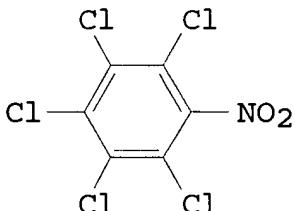
L50 ANSWER 11 OF 13 HCA COPYRIGHT 2002 ACS

90:49449 Study of the fungal resistance of plasticized poly(vinyl chloride). Bochkareva, G. G.; Ovchinnikov,

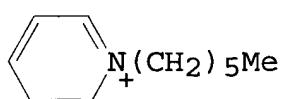
Yu. V.; Kurganova, L. N.; Beirekhova, V. A. (USSR).

Biopovrezhdeniya Mater. Zashch. Nikh, 151-3. Editor(s): Starostin, I. V. Izd. Nauka: Moscow, USSR. (Russian) 1978. CODEN: 39NJAS.

GI



I



Cl⁻

II

AB Penicillium funiculosum decompd. the protective dioctyl adipate [123-79-5] coating supplied as the only C source, forming fumaric acid [110-17-8]. The fungus also decompd. dioctyl sebacinate [2432-87-3], but not dioctyl phthalate [117-84-0] which was resistant even in the presence of sugar. The availability of sugar enhanced formation of enzymes by fungi and stimulated decompn. of PVC [9002-86-2] foils. The destruction of the protective coating by mold decreased the frost resistance of the foils. Only the foils contg. dioctyl phthalate retained their frost resistance after exposure to mold. Opaque clear PVC foils were protected from mold by captan [133-06-2], phthalan [

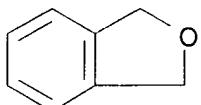
496-14-0], 0.5-1% pentachloronitrobenzene (I) [82-68-8], or 1-2% cetylpyridinium chloride (II) [123-03-5], while transparent foils were protected by 0.1-0.3% bis(tributyltin oxide) [56-35-9] or tributyltin acetate [56-36-0].

IT **496-14-0**

(mold control by, on PVC)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



IT **9002-86-2**

(mold control on)

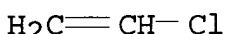
RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4

CMF C2 H3 Cl



CC 5-2 (Agrochemicals)

ST PVC protective coating mold fungicide

IT Penicillium funiculosum

(PVC coatings response to)

IT Mold (fungus)

(control of, on PVC)

IT Fungicides and Fungistats

(for PVC)

IT 117-84-0 123-79-5 2432-87-3

(catabolism of, by mold, PVC degrdn. in relation to)

IT 56-35-9 56-36-0 82-68-8 123-03-5 133-06-2 **496-14-0**

(mold control by, on PVC)

IT **9002-86-2**

(mold control on)

L50 ANSWER 12 OF 13 HCA COPYRIGHT 2002 ACS

89:195587 Effect of storage on pesticide residues in canned food.

Timofeeva, O. A.; Shvartsman, G. A.; Pyshnaya, E. G. (Mold.

Nauchno-Issled. Inst. Pishchevoi Prom., Kishinev, USSR). Konservn.

Ovoshchesush. Prom-st. (9), 10-12 (Russian) 1978. CODEN: KOPRAU.

ISSN: 0023-3587.

AB Hexachlorobutadiene [87-68-3] was very **stable** in canned grape juice during storage for 2 yr. In open cans it disappeared in a few days. γ -Hexachlorocyclohexane [58-89-9] decreased only

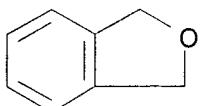
slightly in canned plum compote during 2 yr of storage. Phthalan [496-14-0] decreased to zero in canned grape juice during 4 yr of storage. Carbophos [121-75-5] decreased very slowly in both canned products, whereas Anthio [2540-82-1] decreased rapidly; however, the latter formed the toxic compd. phosphamide [60-51-5], which was **stable**. Therefore, storage of canned juices or compotes is not a dependable method of reducing their fungicide and insecticide residues.

IT 496-14-0

(of canned fruits and juice, storage effect on)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 17-2 (Foods)

Section cross-reference(s): 5

IT 58-89-9 60-51-5 87-68-3 121-75-5 496-14-0

2540-82-1

(of canned fruits and juice, storage effect on)

L50 ANSWER 13 OF 13 HCA COPYRIGHT 2002 ACS

68:28708 Activity of some fungicides on tomato Phytophthora. Granin, E. F.; Izubenko, V. V. Khim. Sel'sk. Khoz., 5(5), 347-51 (Russian) 1967. CODEN: KSKZAN.

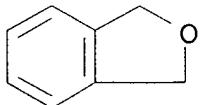
AB Tomato plants 15-18 cm. tall were sprayed with fungicide suspensions (9 .mu.L/cm²) and infected with P. infestans. The most effective fungicides were marzine (total protection by a 0.04% suspension), zineb, figone, captan, and polycarbazine. Kuprazine 1, phthalan, ferbam, and ziram were less effective, while CuCl₂, even when used in high concns. (0.5%), did not give total protection. The loss of activity caused by direct sunlight and moisture was high for marzine, but was smaller for polycarbazine; CuCl₂ was the most **stable** fungicide tested. 14 references.

IT 496-14-0

(Phytophthora infestans control by, on tomatoes)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 19 (Pesticides)

IT 117-80-6 133-06-2 137-30-4 303-25-3 496-14-0

7447-39-4 8065-68-7 9006-42-2 12122-67-7 12427-38-2

14484-64-1

(Phytophthora infestans control by, on tomatoes)

=> d 151 1-7 cbib abs hitstr hitind

L51 ANSWER 1 OF 7 HCA COPYRIGHT 2002 ACS

136:247398 Etherification method for producing benzyl ether derivatives of 2-butene-1,4-diols. Krishnamurti, Ramesh; Wang, Qi; Smolka, Thomas F. (Occidental Chemical Corporation, USA; Stephens, Dinah, H.). PCT Int. Appl. WO 2002022537 A2 20020321, 19 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-GB4036 20010910. PRIORITY: US 2000-PV231790 20000911.

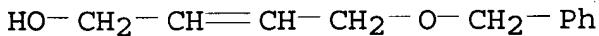
AB A method for producing benzyl ethers of 2-butene-1,4-diols, useful as polymer **stabilizers** (no data), comprises reacting 2-butene-1,4-diols (e.g., 2-butene-1,4-diol) with benzyl chlorides (e.g., benzyl chloride) in the presence of an alkali (e.g., sodium hydroxide) or alk. earth metal hydroxide or carbonate, optionally in the presence of a phase-transfer catalyst (e.g., benzyltriethylammonium chloride) to produce mono- and/or di-benzyl ethers of 2-butene-1,4-diols [e.g., 1,4-bis(benzyloxy)-2-butene] and recovering at least a portion of at least one such benzene deriv.

IT 80885-30-9P

(etherification method for producing benzyl ether derivs. of 2-butene-1,4-diols)

RN 80885-30-9 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



IC ICM C07C041-00

CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 37, 45

IT 70677-94-0P, 1,4-Bis(benzyloxy)-2-butene 80885-30-9P

(etherification method for producing benzyl ether derivs. of 2-butene-1,4-diols)

L51 ANSWER 2 OF 7 HCA COPYRIGHT 2002 ACS

136:102461 **Stability**, Reactivity, Solution, and Solid-State Structure of Halomethylzinc Alkoxides. Charette, Andre B.; Molinaro, Carmela; Brochu, Christian (Departement de Chimie, Universite de Montreal, Montreal, QC, H3C 3J7, Can.). Journal of the American Chemical Society, 123(49), 12160-12167 (English) 2001.

CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB The development of a Lewis acid-catalyzed cyclopropanation of allylic alcs. with bis(iodomethyl)zinc is reported. Iodomethylzinc alkoxides (e.g., chloro- and iodomethyl zinc 4-methoxybenzyloxy compds.) can be formed by treatment of an alc. with bis(iodomethyl)zinc, and their crystal structures solved. These species are not prone to undergo cyclopropanation at low temp., but the addn. of a Lewis acid in catalytic amts. induces the cyclopropanation reaction. Thus, CH₂I₂ and Et₂Zn were stirred and added to cinnamyl alc. in the presence of TiC₄, to give the cyclopropanation product, trans-(3-phenylcyclopropyl)methanol, in ~90% yield. The Lewis acid-catalyzed pathway significantly overwhelms the uncatalyzed one. The prepn. and **stability** of halomethyl zinc alkoxides in soln., their aggregation state in soln., and solid-state structures are discussed. Furthermore, the competition reaction between the inter- vs. intramol. cyclopropanation is studied. Finally, the possible activation pathways to explain the Lewis acid activation of halomethylzinc alkoxides is discussed.

IT 81028-03-7

(Lewis acid-catalyzed cyclopropanation of allylic alcs. with bis(halomethyl)zinc)

RN 81028-03-7 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 29-9 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 75

IT Metal alkoxides

(**stability**, reactivity, soln., and solid-state structure of halomethylzinc alkoxides)

IT 60-12-8, Phenethyl alcohol 67-64-1, Acetone, reactions 75-11-6,
Diiodomethane 100-44-7, Benzyl chloride, reactions 105-13-5,
4-Methoxybenzyl alcohol 122-97-4, 3-Phenyl-1-propanol 556-82-1
557-20-0, Diethyl zinc 928-95-0 1576-95-0 4845-04-9,
1-Cyclohexene-1-methanol 36004-04-3 55131-20-9 75553-23-0
81028-03-7 87770-83-0 388568-84-1

(Lewis acid-catalyzed cyclopropanation of allylic alcs. with bis(halomethyl)zinc)

L51 ANSWER 3 OF 7 HCA COPYRIGHT 2002 ACS

135:272544 One-pot oxidation and Wittig olefination of alcohols using o-iodoxybenzoic acid and **stable** Wittig ylide. Maiti, Arup; Yadav, J. S. (Organic Division, Indian Institute of Chemical Technology, Hyderabad, 500007, India). Synthetic Communications, 31(10), 1499-1506 (English) 2001. CODEN: SYNCAV. ISSN: 0039-7911.

Publisher: Marcel Dekker, Inc..

AB Benzylic, allylic, and propargylic alcs., as well as diols, can be oxidized with o-iodoxybenzoic acid (IBX) in the presence of **stabilized** Wittig ylide to generate .alpha.,.beta.-unsatd. ester in one pot. This is useful when the intermediate aldehydes are unstable and difficult to isolate. For example, to a soln. of benzenemethanol in dimethylsulfoxide was added a mixt. of (triphenylphosphoranylidene)acid Et ester and 2-iodoxybenzoic acid. The yield of Et cinnamate thus prep'd. was 98%.

IT 81028-03-7

(prepn. of .alpha.,.beta.-unsatd. esters by one-pot oxidn. and Wittig olefination of alcs. using iodoxybenzoic acid and (triphenylphosphoranylidene)acetate (Wittig ylide))

RN 81028-03-7 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 21-2 (General Organic Chemistry)

IT 100-51-6, Benzenemethanol, reactions 106-24-1 107-19-7,
2-Propyn-1-ol 107-21-1, 1,2-Ethanediol, reactions 504-63-2,
1,3-Propanediol 821-11-4 1099-45-2,
(Triphenylphosphoranylidene)acetic acid ethyl ester 4407-36-7
4541-14-4 20739-58-6, 2-Octyn-1-ol 64297-64-9, 2-Iodoxybenzoic
acid 81028-03-7

(prepn. of .alpha.,.beta.-unsatd. esters by one-pot oxidn. and Wittig olefination of alcs. using iodoxybenzoic acid and (triphenylphosphoranylidene)acetate (Wittig ylide))

L51 ANSWER 4 OF 7 HCA COPYRIGHT 2002 ACS

135:93426 **Stabilization** of polymers after exposure to oxidation and article manufacture. Wang, Qi (USA). U.S. Pat. Appl. Publ. US 20010007884 A1 20010712, 9 pp., Cont.-in-part of U. S. Ser. No. 272,843. (English). CODEN: USXXCO. APPLICATION: US 2001-761625 20010117. PRIORITY: US 1999-272843 19990319.

AB **Polyvinyl chloride**, **polyvinylidene chloride**, **polycarbonate**, **polyethylene**, **polypropylene**, polyamide, polyimide, polyether, polyester, or polyvinyl acetate contg. .apprx.0.005-10 phr **stabilizer** are resistant to discoloring after exposure to oxidn. PVC contg. 1.34 g **stabilizer** phthalan had initial yellowness value 17.5, after .gamma. radiation 31.9, and after aging 49.5, vs. 18.1, 50.2, and 75.5, resp., for a control without **stabilizer**.

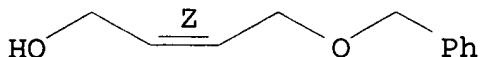
IT 81028-03-7

(**stabilization** of polymers after exposure to oxidn.)

RN 81028-03-7 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 9002-86-2, Poly(vinyl chloride)
) 9002-88-4, Polyethylene 9003-07-0,
Polypropylene
 (stabilization of polymers after exposure to oxidn.)

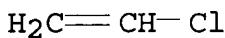
RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4

CMF C2 H3 Cl



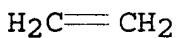
RN 9002-88-4 HCA

CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 74-85-1

CMF C2 H4



RN 9003-07-0 HCA

CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1

CMF C3 H6



IC ICM C08K005-06
 ICS C08K005-46

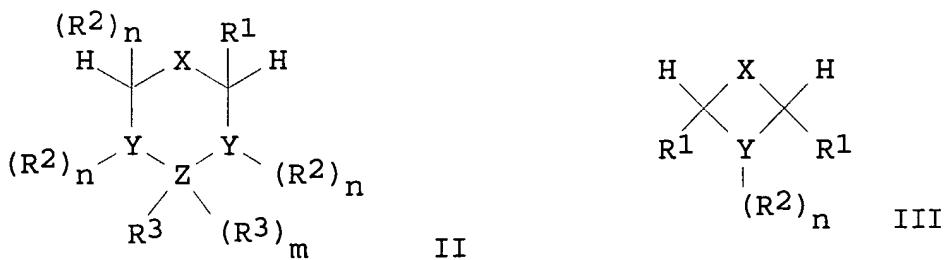
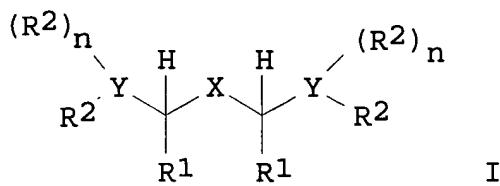
NCL 524083000

CC 37-6 (Plastics Manufacture and Processing)
 ST discoloration prevention agents polymer; PVC phthalan
 stabilizer; polyvinylidene chloride yellowing prevention;
 polycarbonate yellowing prevention; polyethylene
 yellowing prevention; polypropylene yellowing prevention;

polyamide yellowing prevention; polyimide yellowing prevention;
 polyether yellowing prevention; polyester yellowing prevention;
 polyvinyl acetate yellowing prevention
 IT Antioxidants
 Discoloration prevention agents
 Yellowing prevention
 (stabilization of polymers after exposure to oxidn.)
 IT Polyamides, uses
Polycarbonates, uses
 Polyesters, uses
 Polyethers, uses
 Polyimides, uses
Polyurethanes, uses
 (stabilization of polymers after exposure to oxidn.)
 IT 110-65-6, 2-Butyne-1,4-diol 332-77-4 496-14-0, Phthalan
 589-29-7, 1,4-Benzenedimethanol 1606-85-5, 1,4-Bis(2-hydroxy
 ethoxy)-2-butyne 2568-24-3 5417-32-3 10192-64-0 21285-46-1
 67461-24-9 68972-96-3 **81028-03-7**
 (stabilization of polymers after exposure to oxidn.)
 IT 9002-85-1, Poly(vinylidene chloride) **9002-86-2**,
 Poly(vinyl chloride) **9002-88-4**
 , Polyethylene **9003-07-0**, Polypropylene
 9003-20-7, Poly(vinyl acetate)
 (stabilization of polymers after exposure to oxidn.)

L51 ANSWER 5 OF 7 HCA COPYRIGHT 2002 ACS
 133:267624 **Stabilization** and discoloration prevention of
 polymers after exposure to oxidation and antioxidants therefor.
 Wang, Qi (Occidental Chemical Corporation, USA; Stephens, Dinah).
 PCT Int. Appl. WO 2000056812 A1 20000928, 37 pp. DESIGNATED STATES:
 W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
 CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN,
 IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,
 MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
 TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD,
 RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES,
 FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD,
 TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-GB247
 20000128. PRIORITY: US 1999-272843 19990319.

GI



- AB Poly(vinyl chloride), poly(vinylidene chloride), polycarbonates, polyethylene, polypropylene, polyamides, polyimides, polyethers, polyesters, or poly(vinyl acetate) contg. apprx. 0.005-10 phr of a **stabilizer** I, II, or III, where Z is C, P, Sn, Si, or B; X is $-R_1C:CR_1-$, ethynyl, (un)substituted benzene, pyridine, pyrimidine, triazine, furan, pyrrole, thiophene, or naphthalene ring; each Y is independently O, S, or N; each R is independently H, C1-24-alkyl, C6-24-aryl, C7-24-aralkyl; each R1 is independently R, OR, RCO, ROCO, ROCO₂, PR₂, P(OR)₂, PR(OR), NR₂, R₂NCO, R₂NCO₂, SR, halogen, or two R1 groups can form a ring; each R2 is independently R, RCO, ROCO, P(OR)₂, Sn(R)q(OR)_{3-q}, SnRq(OCOR)_{3-q}, Si(R)q(OR)_{3-q}, BRq(OR)_{2-q}, or two R2 groups can form a ring; each R3 is independently R, RCO, ROCO, ROCO₂, OR, SR, NR₂, OPR₂, or OP(OR)₂; m is 0 when Z is P or B and 1 when Z is Sn, Si, or C; n is 0 when Y is O or S and 1 when Y is N; p is 0-4; and q is 0-3 for the tin **stabilizers** and 0-2 for the boron **stabilizers**, with the proviso that in I, when X = $-CH:CH-$, Y = O and R2 = H, at least one of the R1 is not H; and in II, when X = $-R_1C:CR_1-$, Y = O and Z = C, then at least one of the R3 groups on Z is not H. Thus, a plaque from a compn. comprising PVC 150.00, stearic acid 0.30, Mark 152S 0.23, dioctyl phthalate 97.50, Drapex 6.8 15.00, and phthalan 1.34 g was irradiated with 50 kGy gamma-rays, and aged 48 h at 50.degree., giving yellowness 17.5 initially, 31.9 after radiation, and 49.5 after aging, compared with 18.1, 50.2, and 75.5, resp., without phthalan.
- IT 81028-03-7, cis-4-Benzylxy-2-buten-1-ol
 (stabilization and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)
- RN 81028-03-7 HCA
- CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 9002-86-2, PVC 9002-88-4,
Polyethylene 9003-07-0, Polypropylene
 (stabilization and discoloration prevention of polymers
 after exposure to oxidn. and antioxidants therefor)

RN 9002-86-2 HCA
 CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

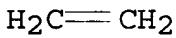
CRN 75-01-4
 CMF C2 H3 Cl



RN 9002-88-4 HCA
 CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

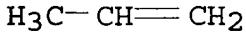
CRN 74-85-1
 CMF C2 H4



RN 9003-07-0 HCA
 CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1
 CMF C3 H6



IC ICM C08K005-00
 ICS C08K005-053; C08K005-15; C08K005-06
 CC 37-6 (Plastics Manufacture and Processing)
 ST antioxidant yellowing prevention polymer; PVC phthalan
 antioxidant gamma radiation; polyolefin antioxidant yellowing
 prevention; vinyl compd polymer antioxidant yellowing prevention;
 polycarbonate antioxidant yellowing prevention;
 polyurethane antioxidant yellowing prevention; polyamide

antioxidant yellowing prevention; polyimide antioxidant yellowing prevention; polyether antioxidant yellowing prevention; polyester antioxidant yellowing prevention

IT Yellowing prevention
 Yellowing prevention
 (agents; **stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT Antioxidants
 (**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT Polyamides, uses
Polycarbonates, uses
 Polyesters, uses
 Polyethers, uses
 Polyimides, uses
Polyurethanes, uses
 (**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT Discoloration prevention agents
 Discoloration prevention agents
 (yellowing; **stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT 110-64-5, 2-Butene-1,4-diol 110-65-6, 2-Butyne-1,4-diol
 332-77-4, 2,5-Dimethoxy-2,5-dihydrofuran 496-14-0, Phthalan
 589-29-7, 1,4-Benzenedimethanol 1606-85-5, 1,4-Bis(2-hydroxyethoxy)-2-butyne 2568-24-3, 4,7-Dihydro-2-phenyl-1,3-dioxepin 10192-64-0 21285-46-1 67461-24-9 68972-96-3, cis-1,4-Bisbenzyloxy-2-butene 70677-94-0 81028-03-7, cis-4-Benzylbenzoate
 (**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT 9002-85-1, Poly(vinylidene chloride) 9002-86-2,
 PVC 9002-88-4, **Polyethylene**
 9003-07-0, **Polypropylene** 9003-20-7, Poly(vinyl acetate)
 (**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

L51 ANSWER 6 OF 7 HCA COPYRIGHT 2002 ACS

131:257029 Deprotection of tetrahydropyranyl ethers with montmorillonite K-10 clay in methanol. Taniguchi, Takahiko; Kadota, Kohei; ElAzab, Adel S.; Ogasawara, Kunio (Pharmaceutical Institute, Tohoku Univ., Sendai, 980, Japan). *Synlett* (8), 1247-1248 (English) 1999. CODEN: SYNLES. ISSN: 0936-5214. OTHER SOURCES: CASREACT 131:257029.

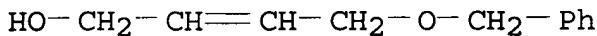
Publisher: Georg Thieme Verlag.

AB A variety of tetrahydropyranyl (THP) ethers are cleaved by montmorillonite K-10 clay in MeOH at room temp. to give the corresponding alcs. THP ethers carrying epoxy, MeOCH₂O, Me₃CPh₂SiO, ACO, and PhCO₂ functionalities are **stable** under the conditions, while ethers carrying ketal, Me₃CMe₂SiO, and Cl₃CC(:NH)O functionalities are unstable.

IT 80885-30-9P

(deprotection of hydroxyl ethers with montmorillonite K-10 in methanol)

RN 80885-30-9 HCA
 CN 2-Buten-1-ol, 4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



CC 21-2 (General Organic Chemistry)

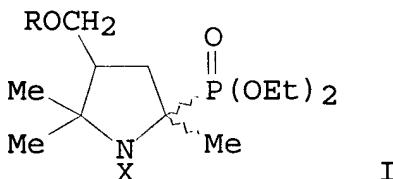
IT 57-88-5P, Cholest-5-en-3-ol (3. β .)-, preparation 89-78-1P
 98-00-0P, 2-Furanmethanol 100-02-7P, 4-Nitrophenol, preparation
 100-51-6P, Benzyl alcohol, preparation 108-95-2P, Phenol,
 preparation 111-70-6P, 1-Heptanol 150-76-5P, 4-Methoxyphenol
 768-95-6P, Tricyclo[3.3.1.13,7]decane-1-ol 1471-15-4P 4541-14-4P
 6318-30-5P 13482-22-9P 32651-37-9P 35435-68-8P 51326-51-3P
80885-30-9P 87184-99-4P 95672-91-6P 101992-89-6P
 130372-07-5P 244298-24-6P 244298-25-7P 244298-46-2P
 244298-47-3P 244781-68-8P

(deprotection of hydroxyl ethers with montmorillonite K-10 in methanol)

L51 ANSWER 7 OF 7 HCA COPYRIGHT 2002 ACS

119:117385 .beta.-Phosphorylated five-membered ring nitroxides:
 synthesis and ESR study of 2-phosphonyl-4-(hydroxymethyl)pyrrolidine aminoxy radical. Stipa, Pierluigi; Finet, Jean Pierre; Le Moigne, Francois; Tordo, Paul (Lab. Struct. React. Espèces Paramagn., Univ. Provence, Marseille, 13397, Fr.). J. Org. Chem., 58(16), 4465-8 (English) 1993. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 119:117385.

GI



AB Intramol. aminomercuration of the alkenyl .alpha.-amino phosphonate PhCH₂OCH₂CH(CMe:CH₂)CH₂CMe(NH₂)P(O)(OEt)₂ followed by sodium borohydride redn. leads to the di-Et [4-(benzyloxymethyl)-2,5,5-trimethylpyrrolidinyl]phosphonate I (R = PhCH₂, X = H). Oxidn. of the phosphonates I (R = H, PhCH₂; X = H) with 3-chloroperbenzoic acid led to the **stable** 2-phosphonylpolyrrolidinyl aminoxy radicals I (same R; X = O.bul.) bearing a 4-(hydroxymethyl) substituent.

IT 81028-03-7

(oxidn. of)
RN 81028-03-7 HCA
CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s) : 22
IT 81028-03-7
 (oxidn. of)

=> d his 161-

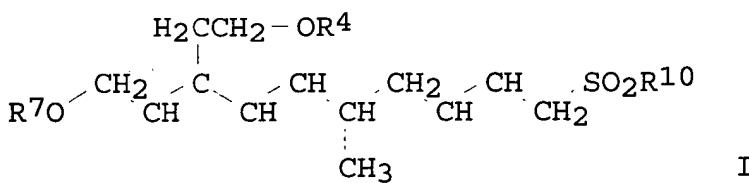
FILE 'LCA' ENTERED AT 17:48:28 ON 28 AUG 2002
L61 14809 S (INHIBIT? OR HINDER? OR IMPED? OR ARREST? OR REDUC? OR
L62 623 S ANTIOXID? OR (ANTI OR INHIBIT? OR HINDER? OR IMPED? OR

FILE 'HCA' ENTERED AT 17:49:47 ON 28 AUG 2002
L63 8 S (L30 OR L31 OR L32) AND L62
L64 5 S L63 NOT (L49 OR L50 OR L51)

```
=> d 164 1-5 cbib abs hitstr hitind
```

L64 ANSWER 1 OF 5 HCA COPYRIGHT 2002 ACS
136:294537 Preparation of bongrekic acid precursors. Shishido, Kozo; Shindo, Mitsuru; Shinohara, Yasuo; Terada, Hiroshi (Foundation for Scientific Technology Promotion, Japan). Jpn. Kokai Tokkyo Koho JP 2002105045 A2 20020410, 35 pp. (Japanese). CODEN: JKXXAF.
APPLICATION: JP 2001-6736 20010115. PRIORITY: JP 2000-224369 20000725.

GI



AB C1-10 segment of bongkrekic acid I (R6, R7 = tert-butylidiphenylsilyl, triisopropylsilyl, tert-butyldimethylsilyl,

triethylsilyl; R10 = lower alkyl, aryl) are prep'd. by reaction of R1COCH₂Me (R1 = substituted 2-oxo-1,3-oxazolidin-3-yl, camphorsultam ring) with X₁CH₂CH:CHCH₂OR₅ (R₅ = corresponding to R₆; X₁ = halo), **redn.**, **oxidn.**, condensation with R₈O_B(OR₉)CHCl₂

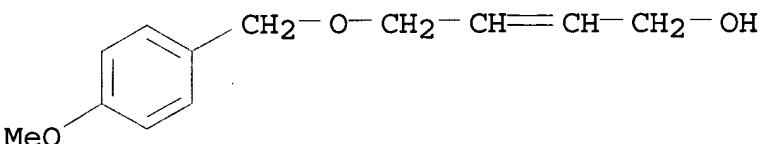
(R₈, R₉ = alkyl, R₈R₉ may form alkylene), coupling reaction with HOCH₂CH:CICH₂CH₂OR₆ (R₆ = same as I), reaction with R₇X₂ (R₇ = same as I; X₂ = halo), deprotection, halogenation, and reaction with R₁₀SO₂M (R₁₀ = lower alkyl, aryl; M = alkali metal). C₁₁-22 segment of bongrekic acid is also manufd. from furanones in eight steps. (2Z,4E,6S,8E)-10-chloro-3-[2-(4-methoxybenzyloxy)ethyl]-1-(methoxymethoxy)-6-methyl-2,4,8-decatriene (prepn. given) was reacted with PhSO₂Na in DMF at room temp. for 20.5 h to give 87% (2Z,4E,6S,8E)-10-phenylsulfonyl-3-[2-(4-methoxybenzyloxy)ethyl]-1-(methoxymethoxy)-6-methyl-2,4,8-decatriene.

IT 409064-73-9P

(prepn. of bongrekic acid precursors)

RN 409064-73-9 HCA

CN 2-Buten-1-ol, 4-[(4-methoxyphenyl)methoxy] - (9CI) (CA INDEX NAME)



IC ICM C07C315-04

ICS C07C317-18; C07C317-22

CC 23-12 (Aliphatic Compounds)

IT 1707-77-3P, 1,2:5,6-Di-O-isopropylidene-D-mannitol 2060-25-5P,

3-Bromo-2-propyn-1-ol 37428-55-0P 76236-32-3P 78508-96-0P,

(S)-5-Hydroxy-2-penten-4-olate 81480-31-1P, (S)-4-Methyl-5-trityloxymethyl-2(5H)-furanone 81677-37-4P, (E)-5-tert-

Butyldiphenylsilyloxy-3-penten-1-yne 112837-18-0P,

(S)-5-Hydroxymethyl-4-methyl-2(5H)-furanone 142860-83-1P

145222-40-8P, 4-(4-Methoxybenzyloxy)-2-butyn-1-ol 146916-76-9P

152126-99-3P, 4-tert-Butyldiphenylsilyloxy-2-buten-1-ol

210056-70-5P, 1-tert-Butyldiphenylsilyloxy-4-iodo-2-butene

397333-59-4P, (E)-1-Bromo-3-tert-butyldiphenylsilyloxy-1-propene

409064-73-9P 409064-74-0P, 1-tert-Butyldiphenylsilyloxy-4-

(4-methoxybenzyloxy)-2-butene 409064-75-1P, 1-Bromo-4-tert-

butyldiphenylsilyloxy-2-butene 409064-76-2P, (Z)-3-Iodo-5-(4-

methoxybenzyloxy)-2-penten-1-ol 409064-87-5P 409064-88-6P

409064-89-7P 409064-90-0P 409064-97-7P, Ethyl

(2E,4Z,6R,10E)-12-tert-butyldiphenylsilyloxy-6-hydroxy-2,5-dimethyl-

2,4,10-dodecatriene-8-ynoate 409064-98-8P, Ethyl

(2E,4Z,6R,10E)-12-tert-butyldiphenylsilyloxy-6-methoxy-2,5-dimethyl-

2,4,10-dodecatriene-8-ynoate 409064-99-9P, Ethyl

(2E,4Z,6R,8Z,10E)-12-tert-butyldiphenylsilyloxy-6-methoxy-2,5-

dimethyl-2,4,8,10-dodecatetraenoate

(prepn. of bongrekic acid precursors)

L64 ANSWER 2 OF 5 HCA COPYRIGHT 2002 ACS

130:227519 Skin care cosmetics containing humectants and rough skin-improving agents. Nanba, Tomiyuki; Kaminuma, Mikiko; Okamoto, Akira; Nakajima, Hideo (Shiseido Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 11035443 A2 19990209 Heisei, 14 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1997-207150 19970716.

AB Skin care cosmetics contg. lower alkyl tetritol ethers as humectants and rough skin-improving agents are claimed. A cosmetic lotion contain propylene glycol 5.0, citric acid 4.0, monomethyl erythritol ether 3.0, 95% ethanol 8.0, POE lauryl ether 2.0, **antioxidants** and preservatives, perfumes and ion-exchanged water to 100%.

IT 81028-03-7P
 (skin care cosmetics contg. humectants and rough skin-improving agents)

RN 81028-03-7 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IC ICM A61K007-48

ICS A61K007-00; A61K009-06

CC 62-4 (Essential Oils and Cosmetics)

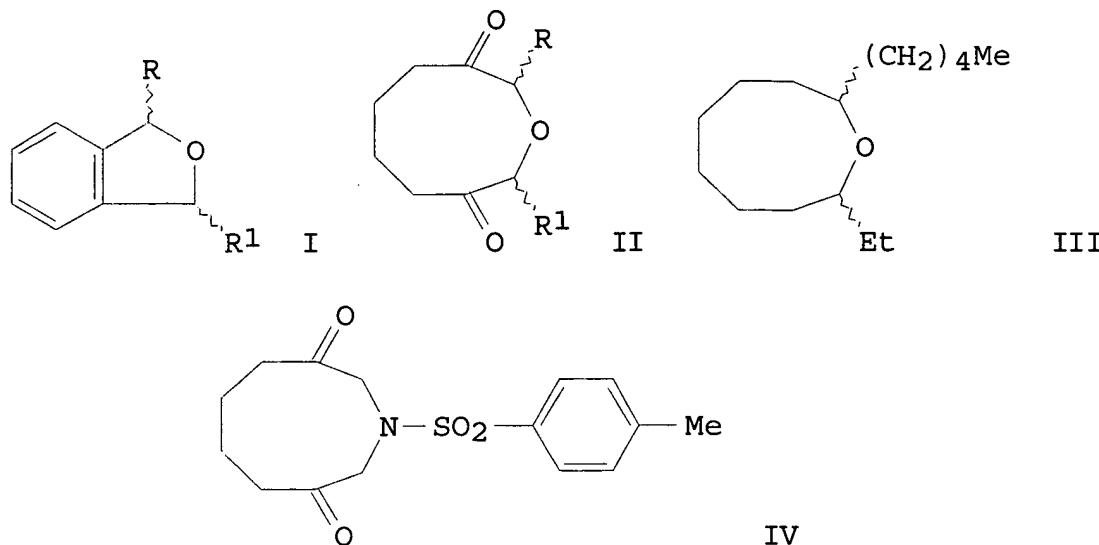
IT 81028-03-7P 85514-70-1P 99903-84-1P 122887-79-0P
 221000-57-3P 221000-58-4P 221000-59-5P 221000-60-8P
 (skin care cosmetics contg. humectants and rough skin-improving agents)

L64 ANSWER 3 OF 5 HCA COPYRIGHT 2002 ACS

120:323072 Preparation of 9-membered cyclic ethers from phthalans.

Synthesis of obtusan. Elliott, Mark C.; Moody, Christopher J. (Dep. Chem., Loughborough Univ. Technol., Loughborough/Leicestershire, LE11 3TU, UK). Synlett (12), 909-10 (English) 1993. CODEN: SYNLES. ISSN: 0936-5214. OTHER SOURCES: CASREACT 120:323072.

GI

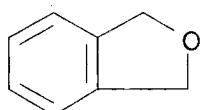


AB Phthalans I [R = R1 = H; R = Et, (CH₂)₄Me, R1 = H; R = (CH₂)₄Me, R1 = Et] have been converted into oxonane-3,8-diones II by a 3-step sequence involving Birch **redn.**, hydrogenation and **oxidative** cleavage; the 2-ethyl-9-pentyl deriv. III [R = (CH₂)₄Me, R1 = Et] has been deoxygenated to give obtusan III. The method was extended to the prepn. of azonane IV from isoindoline.

IT 496-14-0, Phthalan
(reactant, in prepn. of nine-membered cyclic ethers from phthalans and synthesis of obtusan)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



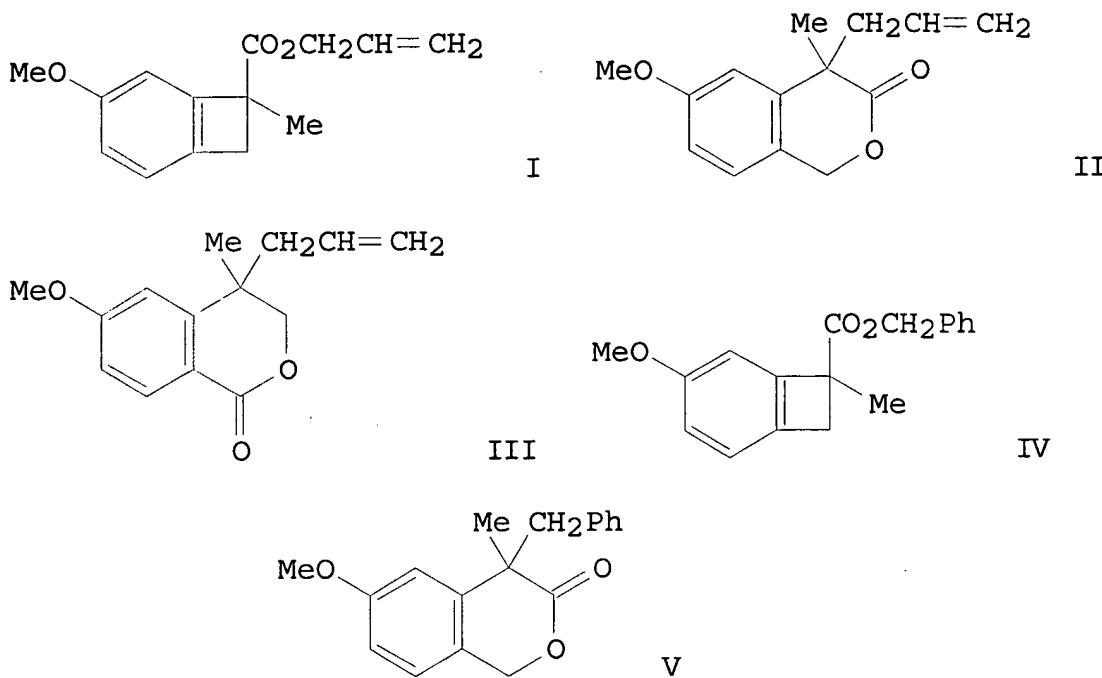
CC 26-9 (Biomolecules and Their Synthetic Analogs)
IT 496-12-8, Isoindoline 496-14-0, Phthalan 628-17-1,
Pentyl iodide

(reactant, in prepn. of nine-membered cyclic ethers from phthalans and synthesis of obtusan)

L64 ANSWER 4 OF 5 HCA COPYRIGHT 2002 ACS

103:215122 Tandem electrocyclic-sigmatropic reaction of benzocyclobutenes. An expedient route to 4,4-disubstituted isochromanones. Shishido, Kozo; Shitara, Eiki; Fukumoto, Keiichiro; Kametani, Tetsuji (Pharm. Inst., Tohoku Univ., Sendai, 980, Japan). J. Am. Chem. Soc., 107(20), 5810-12 (English) 1985. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 103:215122.

GT



AB A novel and useful tandem electrocyclic-sigmatropic reaction of benzocyclobutenes was described. The thermolysis of 1-alkyl-1-carballyloxybenzocyclobutenes e.g. I, readily derivable from 1-cyanobenzocyclobutene, gave 4-alkyl-4-allyl-isochroman-3-ones, e.g. II, via a tandem electrocyclic-[3,3]sigmatropic reaction in excellent yields. II was converted quant. to the isochroman-1-one III by a two-step **redn.-oxidn.** sequence. Thermolysis of 1-alkyl-1-carbobenzyloxybenzocyclobutenes e.g. IV gave 4-alkyl-4-benzylisochroman-3-ones, e.g. V, via a tandem electrocyclic-[1,3]sigmatropic reaction. Those results provide a general and efficient procedure for constructing the isochromanones with quaternary carbon on a benzylic carbon. The isochromanones are synthons for Amaryllidaceae alkaloids.

IT 69152-88-1 81028-03-7

(esterification by, of benzocyclobutene carboxylic acid deriv.)

RN 69152-88-1 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 81028-03-7 HCA
 CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

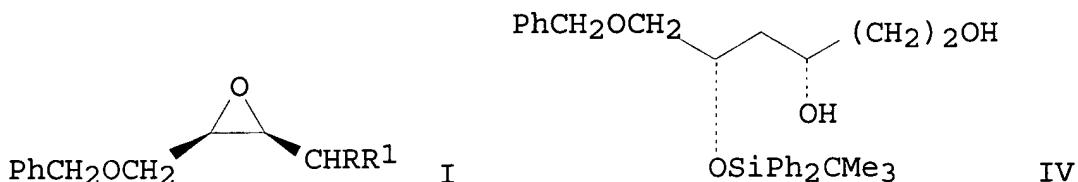
Double bond geometry as shown.



CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 31
 IT 100-51-6, reactions 105-13-5 107-19-7 586-98-1 636-72-6
 2028-63-9 21964-44-3 51410-44-7 69152-88-1
81028-03-7
 (esterification by, of benzocyclobutene carboxylic acid deriv.)

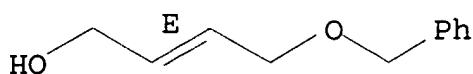
L64 ANSWER 5 OF 5 HCA COPYRIGHT 2002 ACS
 98:88772 Stereocontrolled synthesis of 1,3,5... (2n + 1) polyols.
 Nicolaou, K. C.; Uenishi, J. (Dep. Chem., Univ. Pennsylvania,
 Philadelphia, PA, 19104, USA). J. Chem. Soc., Chem. Commun. (22),
 1292-3 (English) 1982. CODEN: JCCCAT. ISSN: 0022-4936.

GI



AB The stereoselective prepn. of 1,3,5... (2n + 1)-polyols based on the Sharpless asym. epoxidn. and regioselective ring opening by (Me2CHCH2)2AlH is reported. E.g., epoxidn. of (E)-PhCH2OCH2CH:CHCH2OH with Me3COOH in CH2Cl2 contg. Ti(OCHMe2)4 and di-Et (-)-tartrate at -23.degree. gave 80% epoxide I (R = H, R1 = OH) which on oxidn. and Wittig reaction with Ph3P:CHCO2Me gave I (RR1 = CHCO2Me) (II) as a 84:16 E:Z mixt. Ring opening of II with (Me2CHCH2)2AlH in CH2Cl2 at -78.degree. and protection of the hydroxyl group gave PhCH2OCH2CH(OSiPh2CMe3)CH2CH:CHCH2OH (III). Epoxidn. of III as above followed by redn. with NaAl2(OCH2CH2OMe)2 in THF at 0-25.degree. gave alc. IV.
 IT 69152-88-1
 (epoxidn. of, stereospecific)
 RN 69152-88-1 HCA
 CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 23-7 (Aliphatic Compounds)

Section cross-reference(s): 27, 33

IT 69152-88-1

(epoxidn. of, stereospecific)

IT 84582-67-2P

(prepn., epoxidn., redn., oxidn., and Wittig reactions of)